# Chemical reaction

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A **chemical reaction** is a process involving one, two or more substances (called reactants), characterized by a chemical change and yielding one or more product(s) which are different from the reactants. Classically, chemical reactions encompass changes that strictly involve the motion of electrons, although the general concept of a chemical reaction (in particular the notion of a chemical equation) is applicable to transformations of elementary particles, as well as nuclear reactions.

## Contents



## Types

There are five major classifications of chemical reactions. Some common and widely known are:

- Isomerization (**A → B**) in which a compound undergoes a structural rearrangement without any change in its net atomic composition;
- Direct combination or synthesis (**A + B → C**), in which two or more elements or compounds unite to form a more complex product;
- Chemical decomposition or analysis (**A → B + C**), in which a compound is decomposed into smaller compounds;
- Single displacement or substitution (**A + BC → AC + B**), characterized by an element being displaced out of a compound by a more reactive element;
- Double displacement or substitution (**AC + BD → AD + BC**), in which two compounds in aqueous solution (usually ionic) exchange elements or ions to form different compounds.

The collision of more than two particles into the ordered structure necessary to perform chemical transformations is extremely unlikely; which is why ternary reactions in practice are not observed. A chemical reaction may require three or more reagents, but the process can generally be decomposed into a stepwise series (or a a set of stepwise series) of the above.

The large diversity of chemical reactions makes it difficult to establish simple criteria for functional (as opposed to mechanistic) classification. However, some kinds of reactions have similarities which make it possible to define some larger groups. A few examples are:

- organic reactions, which encompass several different kinds of reactions involving compounds which have carbon as the main element in their molecular structure.

- redox reactions, which involve augmenting or decreasing the electrons associated with a particular atom.
- Combustion, where a substance reacts with oxygen gas;

See list of reactions for more examples.

# Energy and reactions

## Net change in energy

According to the Third law of thermodynamics, any closed system will tend to minimize its free energy. Without any outside influence, any reaction mixture, too, will try to do the same. For many cases, an analysis of the enthalpy of the system will give a decent account of the energetics of the reaction mixture. The enthalpy of a reaction is calculated using standard reaction enthalpies and Hess' law of constant heat summation. Many of these enthalpies may be found in beginners' books on thermodynamics. For example, consider the reaction

$$CH_4 + 2\ O_2 \rightarrow CO_2 + 2\ H_2O$$

(combustion of methane in oxygen). By calculating the amounts of energy required to break all the bonds on the left ("before") and right ("after") sides of the equation using collected data, it is possible to calculate the energy difference between the reactants and the products. This is referred to as $\Delta H$, where $\Delta$ (Delta) means difference, and $H$ stands for enthalpy, a measure of energy which is equal to the heat transferred at constant pressure. $\Delta H$ is usually given in units of kilojoules (kJ) or in kilocalories (kcal).

### Exothermic reactions

If $\Delta H$ is negative for the reaction, then energy has been released often in the form of heat. This type of reaction is referred to as exothermic (literally, outside heat, or throwing off heat). An exothermic reaction is more favourable and thus more likely to occur. An example reaction is combustion, which we already know from everyday experience, since burning gas in air produces heat.

### Endothermic reactions

A reaction may have a positive $\Delta H$. If a reaction has a positive $\Delta H$, it consumes energy as the reaction moves towards completion. This type of reaction is called endothermic (literally, inside heat, or absorbing heat).

## Exceptions to the rule

The above rule, "Exothermic reactions are favourable", is usually true. However, there may be situations where exothermic reactions may not be favourable. This happens when the stability obtained due to loss of enthalpy is off set by a corresponding decrease in entropy (a measure of randomness). The exact rule is that a reaction is favourable when the Gibbs free energy of that reaction is negative where $\Delta G = \Delta H - T\Delta S$; $\Delta G$ being the change in Gibbs free energy, $\Delta H$ being the change in enthalpy, and $\Delta S$ is the change in entropy

## Reactive intermediates

While Thermodynamics attempts to answer the question: "Will this reaction occur?", another important question "How fast is the reaction?" is left completely unanswered by it. This is because Thermodynamics (or what is now known as Equilibrium Thermodynamics) tries to understand the reaction in terms of the initial and final states of the reaction mixture. It does not attempt to figure out the process by which a reaction occurs. This field of study is

taken up by the field of Reaction Kinetics Reactions very seldom occur directly. Usually, reactants must collide to form an activated complex. This has a higher internal energy than the original reactants combined, having gained some from the kinetic energy of the collision. This energy allows for the rearrangement of bonds which constitutes the reaction. In some reactions, the reactants may pass through several reactive intermediates before becoming products. Reaction Kinetics attempts to put all these phenomena into perspective.

# Reaction Rate

The rate of a chemical reaction is a measure of how concentration of the involved substances changes with time. Analysis of reaction rates is important for several applications, such as in chemical engineering or in chemical equilibrium study. Rates of reaction depends basically on:

- Reactant concentrations, which usually make the reaction happen at a faster rate if raised,
- Activation energy, which is defined as the amount of energy required to make the reaction start and carry on spontaneously. Higher activation energy implies that a reaction will be harder to start and, therefore, slower.
- Temperature, which hastens reactions if raised, because higher temperature means that the involved species will have more energy, thus making the reaction easier to happen,
- The presence or absence of a catalyst. Catalysts are substances which increases the speed of a reaction by lowering the activation energy needed for the reaction to take place. A catalyst is not destroyed or changed during a reaction, so it can be used again.

Reaction rates are related to the concentrations of substances involved in reactions, as quantified by the law of mass action.

# Reversibility and spontaneity

Every chemical reaction is, in theory, reversible. In a *forward reaction* the substances defined as reactants are converted to products. In a *reverse reaction* products are converted into reactants.

Chemical equilibrium is the state in which the forward and reverse reaction rates are equal, thus preserving the amount of reactants and products. However, a reaction in equilibrium can be driven in the forward or reverse direction by changing reaction conditions such as temperature or pressure. Le Chatelier's principle can be used to predict whether products or reactants will be formed.

Although all reactions are reversible to some extent, some reactions can be classified as irreversible. An *irreversible reaction* is one that "goes to completion." This phrase means that nearly all of the reactants are used to form products. These reactions are very difficult to reverse even under extreme conditions.

A reaction is called spontaneous if its thermodynamically favoured, by that meaning that it causes a net increase on global entropy. Spontaneous reactions (in opposition to non-spontaneous reactions) do not need external perturbations (such as energy supplement) to happen. In a system at chemical equilibrium, it is expected to have larger concentrations of the substances formed by the spontaneous direction of the process.

# See also

- Quantum electrochemistry
- Chemical synthesis
- Chemical equation
- List of reactions

- Thermodynamics
- Thermochemistry
- Chemical kinetics



Categories: Chemical reactions